Hypergolic Ignition of Ionic Liquids

IGNITION TEAM

Tom Hawkins, Task Manager

Angelo Alfano, Experimental

Ghanshyam Vaghjiani, Experimental

Jeff Mills, Modeling

Stefan Schneider, Synthesis

Propellant Development Group

Propellants Branch

Air Force Research Laboratory

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE **APR 2005**	2. REPORT TYPE	3. DATES COVERED **-**
4. TITLE AND SUBTITLE **Hypergolic Ignition of Ionic Liquids**		5a. CONTRACT NUMBER
		5b. GRANT NUMBER
		5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S) **Angelo Alfano; Ghanshyam Vaghjiani; Jeffrey Mills**		5d. PROJECT NUMBER **2303**
		5e. TASK NUMBER **0423**
		5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Air Force Research Laboratory (AFMC),AFRL/PRSP,10 E. Saturn Blvd.,Edwards AFB,CA,93524-7680**		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR’S ACRONYM(S)
		11. SPONSOR/MONITOR’S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT
N/A

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**		**15**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

IGNITION TEAM
Personnel and Support

TEAM LEADER

Support

AFOSR

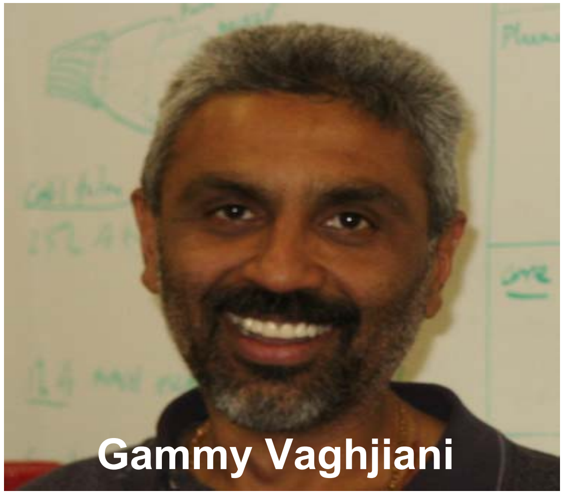
AFRL

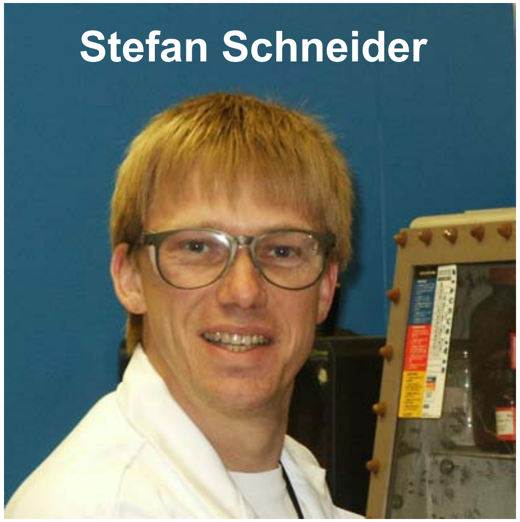
Propulsion Division

Spacecraft Branch

Theoretician

Experimentalists





Hypergolic Ignition of Ionic Liquids

IGNITION SURVEY DOCUMENT WRITTEN

- EVALUATED 13 IGNITION TECHNIQUES FOR IL APPLICATIONS & REVIEWED PUBLISHED/FUNDED WORK
- EXPERIMENTAL/COMPUTATIONAL FOCUS ON IL HYPERGOLIC IGNITION; TWO YR (FY05-06) PLAN WRITTEN

HYPERGOLIC IGNITION WORK HAS BEGUN

- OVER 50 VISUAL IGNITION TESTS OF WFNA, IRFNA, and N_2O_4 WITH HYDRAZINES, AMINES, STRAINED-RING HYDROCARBONS, TRIAZOLES, TRIAZOLIUM SALTS, AND FORMULATIONS
- AB INITIO CALCULATIONS OF DECOMPOSITION OF HYDRAZINES, 1,2,3 AND 1,2,4 TRIAZOLES AND THEIR AMINATED DERIVATIVES BY N_2O_4.

RESONANT PHOTOPHYSICAL IGNITION OF HAN-BASED PROPELLANTS

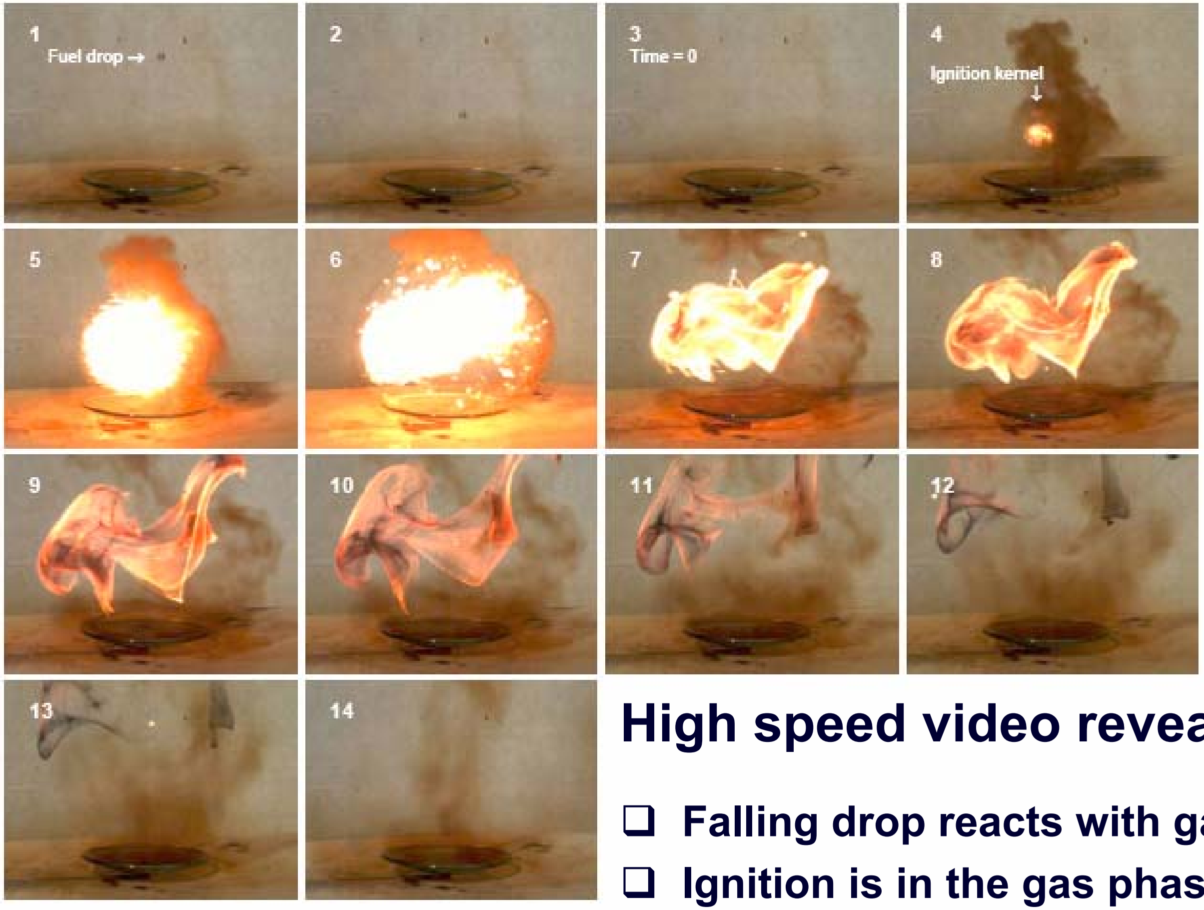
- SINGLE PULSE CO_2 LASER IGNITION DEMONSTRATED DURING AFRL INTERNAL PROJECT

Hypergolic Ignition of Ionic Liquids

GOAL: Develop Capability to Experimentally Determine and Theoretically Validate Hypergolic Ignition Mechanisms in ILs

Technical Challenge:		**Approach:**
Chemical dynamics and mixing dynamics strongly influence hypergolicity and must be decoupled	→	Combine time-resolved techniques (FTIR, emission spectrosc., laser probing, …) with novel reactant mixing strategies
Dozens of simultaneous, unmeasured reaction rates have the potential to control the ignition delay	→	Combine and extend quantum chemical and kinetics codes to focus experimental search for key transients and rate limiting steps

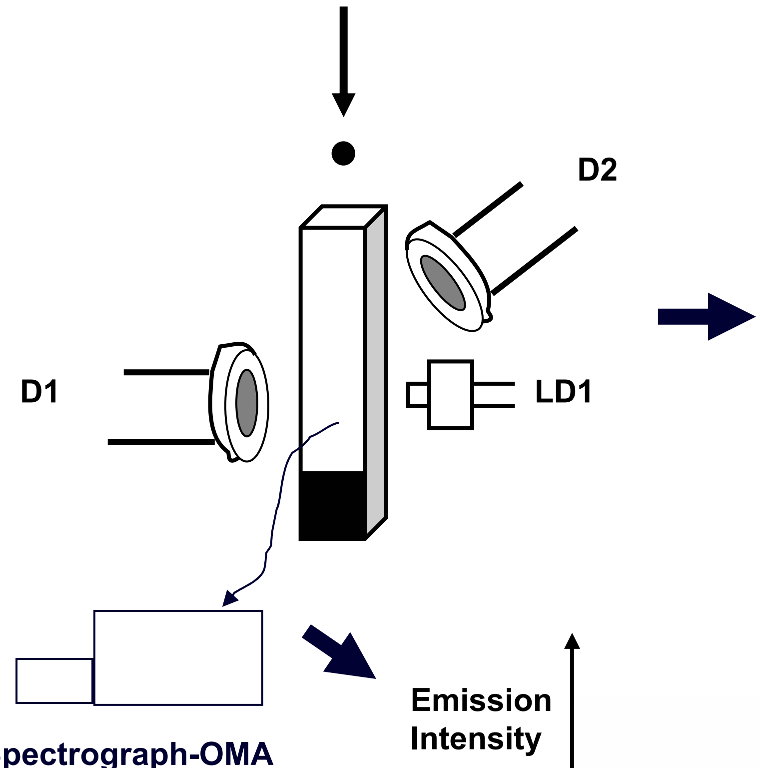
High Speed Video Highlights Complexity

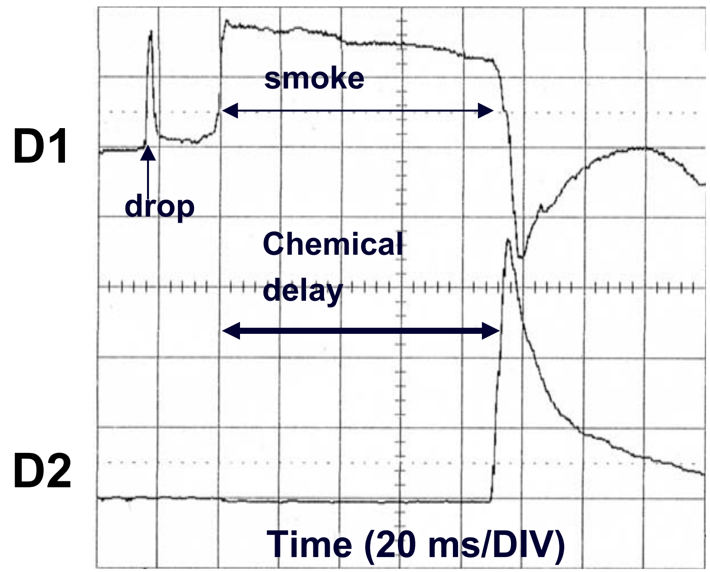


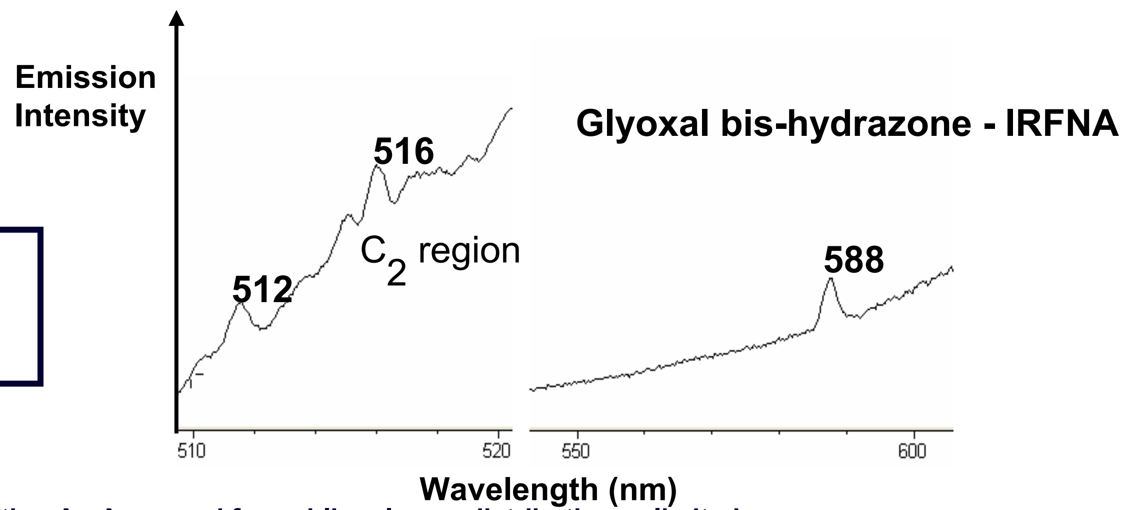
High speed video reveals:

- ❑ Falling drop reacts with gas environment
- ❑ Ignition is in the gas phase
- ❑ Gas phase and liquid phase chemistry is connected
- ❑ Spatially indiscriminate information will not be sufficient for mechanistic understanding

Spatially Resolved Approach Required







COMPLEXITY HIGHLIGHTED IN HIGH SPEED VIDEO IGNORED

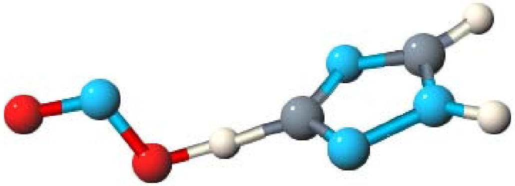
Current Focus

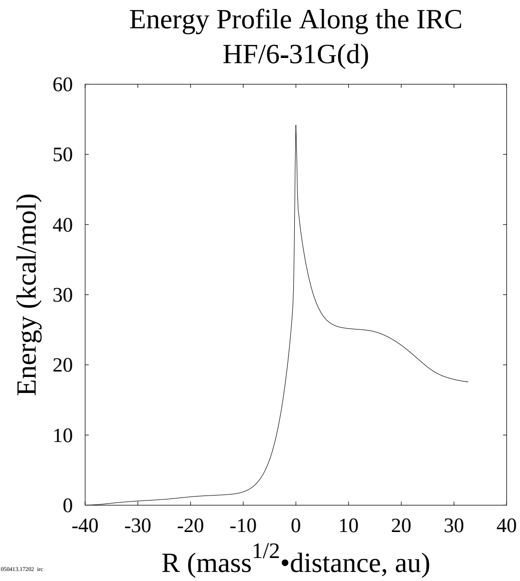
- SIMPLIFY PROBLEM TO LIQUID PLUS GAS

- APPLY SPECTROSCOPIC TOOLS IN THIS REGIME
  - FTIR (RAPID & STEP SCAN)
  - TIME-RESOLVED RAMAN
  - TIME-RESOLVED EMISSION
  - HIGH SPEED VIDEO

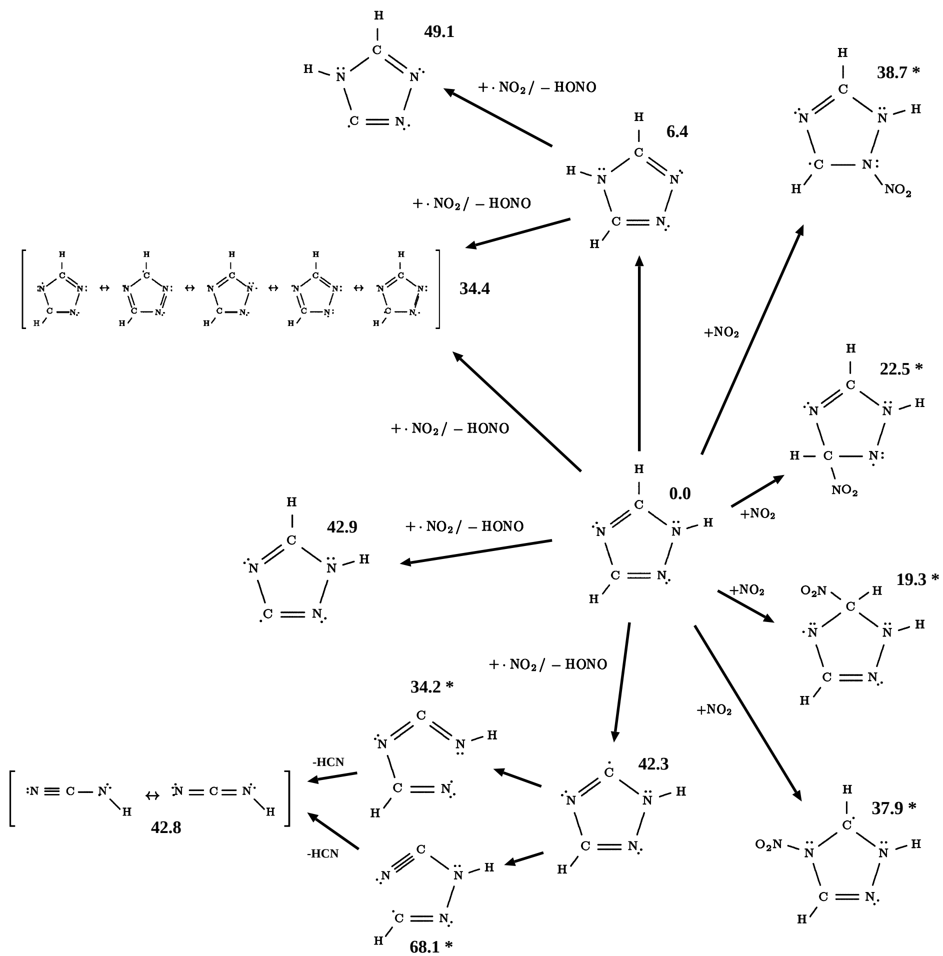
Theory and Modeling

- **Kinetic Parameters** → **Kinetic Model**
- **PES** → **Kinetic Parameters**
- **Reaction Step** → **PES**
- **Net Rxn Enthalpy** → **Reaction Step**
- **Trial Rxn Step** → **Net Rxn Enthalpy**



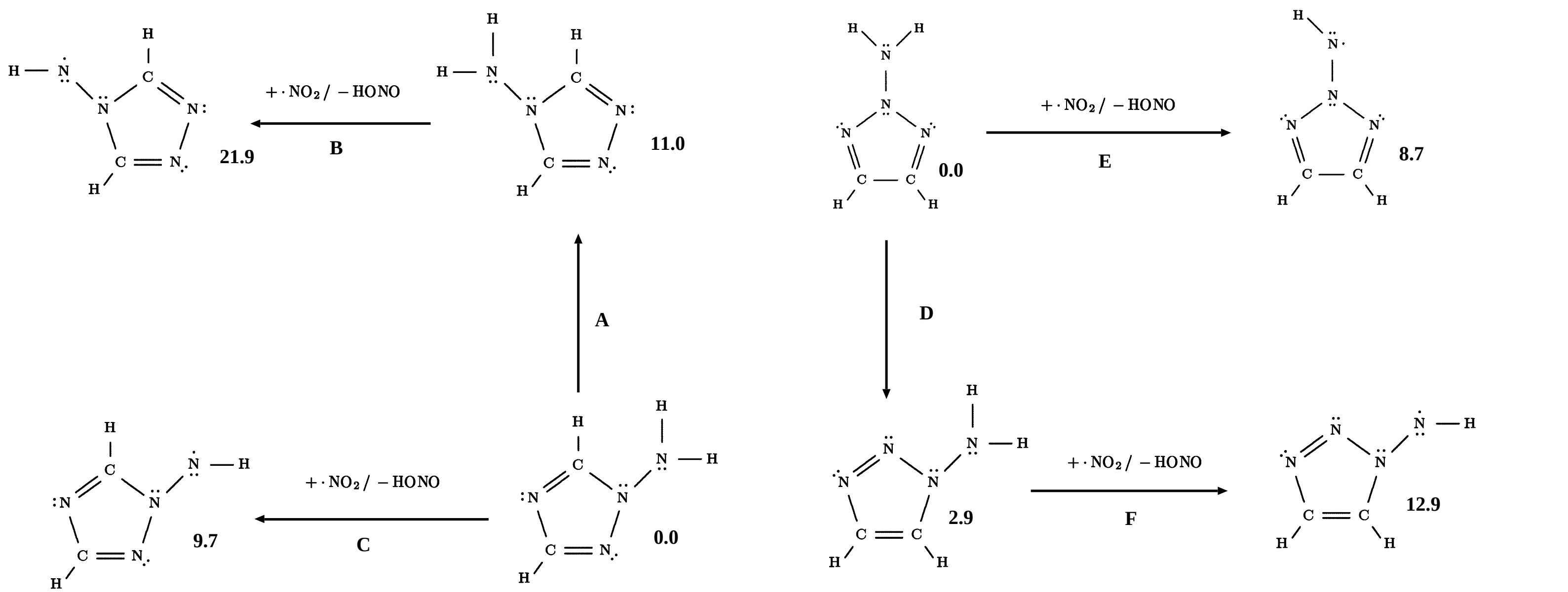


1,2,4-Triazoles + N_2O_4



Distribution A: Approved for public release; distribution unlimited.

Amino-Triazoles + N_2O_4



- Reaction Enthalpies Slightly Above Hydrazine and MMH
- Reaction Enthalpies Correlate with Visual Ignition Tests

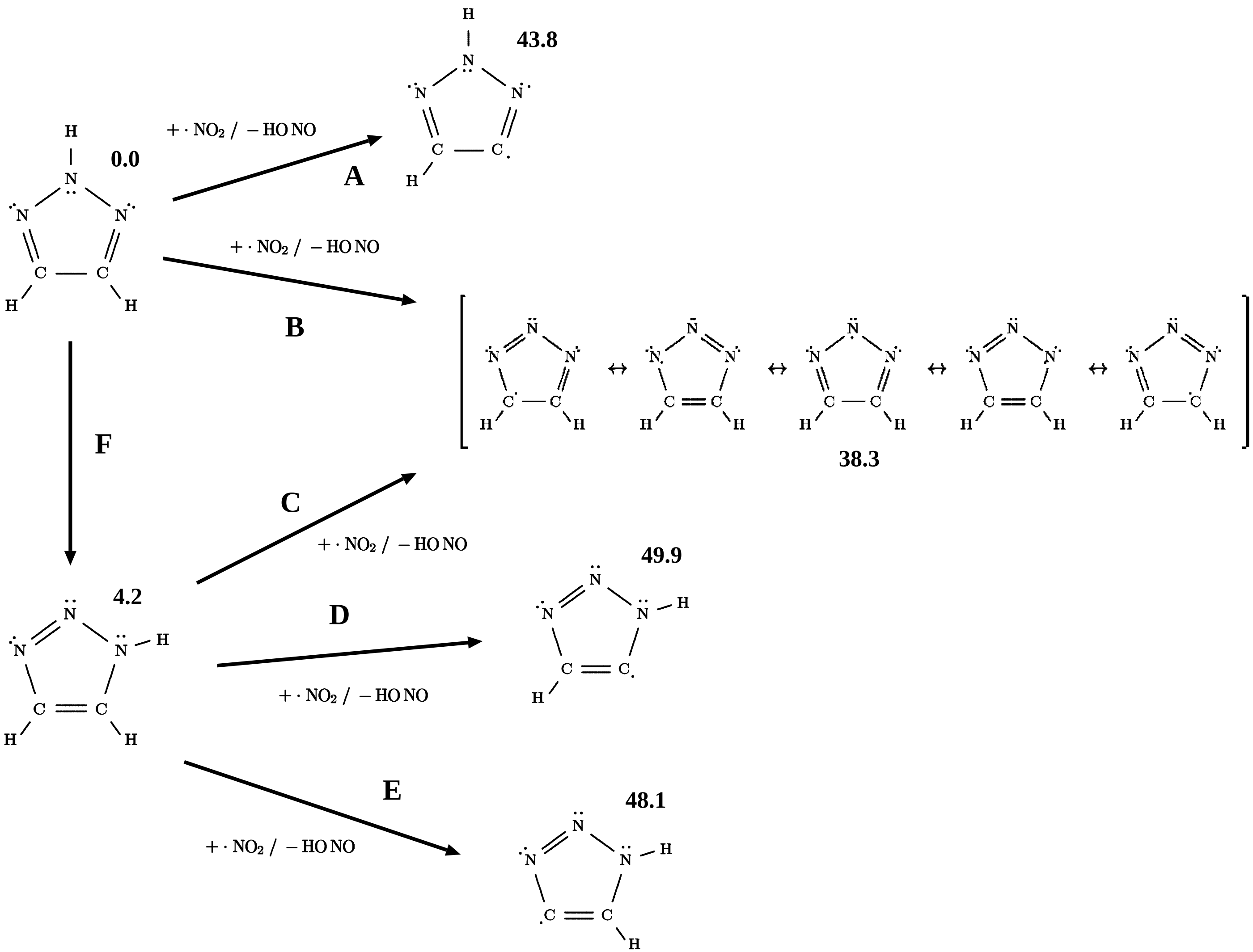
Plan

Develop Capability to Experimentally Determine and Theoretically Validate Hypergolic Ignition Mechanisms in ILs

- **To provide a roster of hypergolicity of IL-oxidizer pairs**
- **To provide ignition mechanisms for a reference set of IL-oxidizer reactions with time-resolved spectroscopic techniques**
- **To provide theoretical validation/prediction for experimental results**
- **To provide a predictive model to suggest targets and screen IL synthesis candidates**

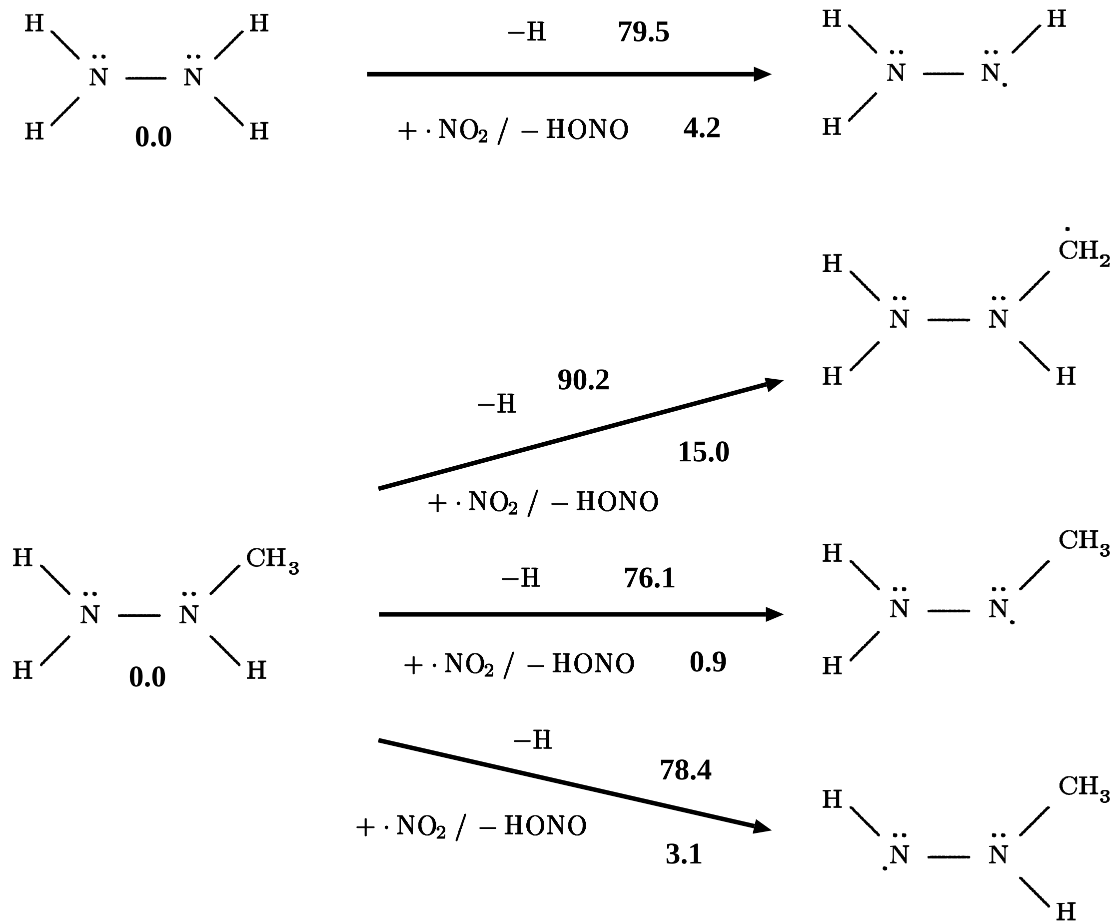
Back-up Slides

1,2,3-Triazoles + N_2O_4



Distribution A: Approved for public release; distribution unlimited.

Hydrazine and MMH



“Potentially Planar” CN Heterocycles

$$\mathrm{Rh}^{\ominus} \xrightarrow{+\mathrm{H}^{\oplus}} \mathrm{R} \xrightarrow{+\mathrm{H}^{\oplus}} \mathrm{RH}^{\oplus} \xrightarrow{+2\mathrm{e}^{\ominus}} \mathrm{RH}^{\ominus} \xrightarrow{+\mathrm{H}^{\oplus}} \mathrm{RH}_2 \xrightarrow{+\mathrm{H}^{\oplus}} \mathrm{RH}_3^{\oplus}$$